

Study of the magnetic anisotropy in a planar model of the La_2CuO_4

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We study the anisotropy energy in a planar model for the $\text{Cu} - \text{O}$ layers of the La_2CuO_4 investigated in previous works. The Tight-Binding (TB) potential of the model was extended out of the validity region with the purpose of incorporate it in the potential. Next, the spin-orbit operator was considered in the Hartree Fock solution of the full HF problem. It follows that in spite of the fact that the extended potential possesses the square symmetry of the crystalline structure, the anisotropy energy vanishes in its purely 2D formulation. The result indicates that for the prediction by the model of the observed non vanishing magnetic anisotropy at zero doping and temperature in La_2CuO_4 , its formulation requires of a 3D representation of its Wannier orbitals and the use of d like orbitals. The consideration of more realistic 3D character of the model, by including multiple CuO planes, also could be important due to the argued absence of long range order in 2D.

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I. INTRODUCTION

The superconductivity is the intrinsic capacity of certain materials that allows to conduct electric currents without resistance and losses of energy in specific conditions. In 1911 it was discovery by Heike Kamerlingh Onnes[1] when observed the electric resistance of the mercury disappear abrupt at 4.2K. In the next years several materials were discovered showing the occurrence of this phenomenon below certain critical temperature value T_c . A microscopic explanation was not arrived until 1960, when Bardeen, Schrieffer and Cooper proposed a successful theory, today known as the BCS theory.

With the discovery of the La_2CuO_4 superconductor in 1986 at $T_c = 30\text{K}$, was open a new stage, up to now devoted to the obtaining and investigation of such kind of high T_c superconductors. In this case, up to nowadays it had not been possible to develop a full explanation for high temperature superconductivity.

The essential characteristic of the first discovered HTc superconductor La_2CuO_4 , and various others in its class, is that it has a crystalline structure containing CuO_2 layers, inside a perovskite structure separated by block layers, who play a main role as charge reservoirs. Usually, the block layers are insulators and do not have any contribution to the low energy electronics states. On another hand in the CuO_2 layers, the minimum energy of the electronics state are around the Fermi level.

At half filling (hole concentration $p=0$), the cuprates are antiferromagnetic insulators (AFI), with a Neel temperature near 300 K. When the number of holes grow, the antiferromagnetic phase is rapidly destroyed and the cuprates show a pseudogap phase. If you continue doping with hole, the metallic phase turns up.

In 1930 Bloch and Wilson [3] developed the band theory, that explain why several materials are metals and another are insulators. However the band theory failed in trying to explain the electronic structure of a large number of insulators. In this group were the NiO , CoO and $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, which were predicted as having metallic behavior. This result opened the doors for the profound study of the strongly correlated materials, which are characterized by showing strong correlation properties among the electrons. Two of the founding fathers of these studies Mott and Hubbard, attributed the insulator behavior to the electron-electron correlation.

Nowadays, a generalized criterion exists: For getting behaviors like the ones of insulators of Mott, it is necessary to take into account the short range correlations between electrons of opposite spin which are included in the phenomenological Hubbard models [4, 5]. It is also clear that the HF approximation, when is considered from first principles in a elemental electronic system, should not be able to predict the correlation between opposite spin electrons. In the recent works [6, 7] by using a one band model, solved in the HF approximation, it was obtained a gap at $T = 0$ for the La_2CuO_4 , then predicting its insulator behavior. This reflect that some of the important properties of these materials, that are products of the strong electronic correlations, can be predicted by the model in the HF approximation. This outcome does not result strange, after taking in mind that, by example the antiferromagnetism, that is a strong correlation property, can be derived form a HF solution of the Hubbard model. The main point to note in this, is that the considered model is not the original first principle electronic system. In fact the model only differs from a Hubbard one in that the near neighbor approximation was not taken.

Since the Hamiltonian adopted in the model does not includes the spin, the HF solution do not determine a direction for the antiferromagnetism. This fact define the basic motivation of this work. It consists in including the spin-orbit interaction in the starting Hamiltonian and then study the effect of the spin-orbit interaction in the solutions. The

expectation was to study the magnetic anisotropy of the model. Therefore, the specific objectives of our work are the following ones:

1. Obtain the form of the spin-orbit operator in the frame of the mentioned model for the superconductor material [6, 7].
2. Afterwards, to evaluate the anisotropy energy of the antiferromagnetic HF states of the model, in the no doping limit of the La_2CuO_4 . For this purpose the mean value of the spin-orbit operator of the electrons with the crystalline field [6, 7] is evaluated in the HF states. Since the HF solution is degenerated with respect to spin rotations, to evaluate the mean value, the HF states were arbitrarily rotated in the spin structure of their many particles [6, 7], by unitary transformations. These spin rotations are the ones representing corresponding space rotations around an arbitrary spatial axis.

II. La_2CuO_4 SYSTEM

In general, the HTSCs presents a tetragonal structure, and have one or more planes CuO_2 in its structure separated by layers of another atoms (Ba, O, La,...). In the CuO_2 planes, each cooper ion is coupled to four oxygen ions separated an approximate distance of 1.9 Å. The critical temperature depended of the maximum number of adjoint layers CuO_2 (figure 1). The electronic behavior of the cuprates is very strongly determined by the electronic density in the two dimensional layers CuO_2 . The basic behavior of the CuO_2 layers, is common for all the cuprate superconductors.

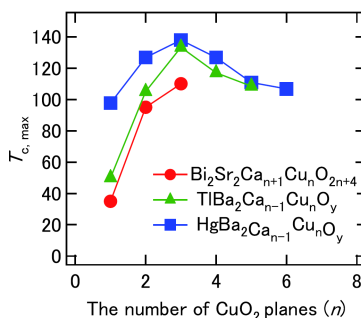


FIG. 1: Dependence of T_c of the HTSC with the number of serial planes CuO_2 .

A. Crystalline structure and phases diagrams

The family of monolayer compounds, $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, where x indicates the magnitude of strontium (Sr) doping, crystallize to the tetragonal structure centered in body (bct), usually named T structure, showed in the figure 2. In the $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ the planes CuO_2 are separated by ~ 6.6 Å, separated by 2 planes of LaO , that act like charge reservoirs, absorbing electrons of the conductor planes under the doping of the material with holes.

Exist consensus in consider the electronic structure of the $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, as quasi two dimensional. This low dimensionality of this electronic system allows to be treated from another viewpoint. For example collective phenomena, such as fluctuations in spin density waves (S.D.W) and charge density waves (C.D.W), could be the origin of the superconducting mechanism [8, 9].

In the figure 3, it is illustrated the phase diagrams in the (x,T) plane for the compound $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, where T is the temperature. Even when the absolute antiferromagnetic order and the insulator Mott state persist for a wide range of temperatures, it is very sensible at doping. For example, in the $T = 0$ limit, it is lost at $x = 0.04$ doping, but in the pseudogap (SG) phases and superconductor (SC) ones, exist experimental evidence of a less extended AFM order [10, 11]. All the ideas mentioned before support the possibility that the AFI state ($x=0$) play a crucial role in guaranteeing first: a correlation between pairs of holes (SG), second: a condensation of these holes toward the SC state [12].

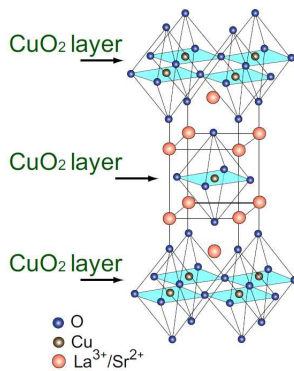


FIG. 2: Crystalline structure of the La_2CuO_4

In this compound a structural phase transition occurs. At high temperatures the structure is tetragonal, but for low temperature the Cu atoms and the six oxygens around them, stray slowly of their positions, forming an orthorhombic structure. In the majority of the theoretical studies about this compound, this little distortion is usually ignored.

The crystalline structure of the LSCO have simple CuO_2 planes, while the systems $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+y}$ and $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO) has double CuO_2 planes. The intermediate layers of LSCO do not have the Cu–O chains that affects considerably the CuO_2 planes, in contrast with YBCO, and the complicate structure that present the intermediate layers of the Bi_{2212} .

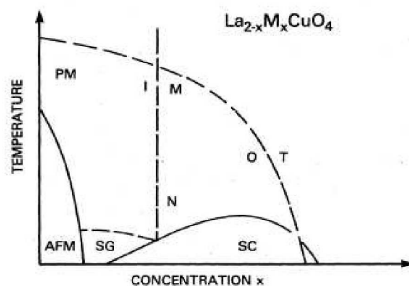


FIG. 3: Phases diagram of the $\text{La}_{2-x}\text{M}_x\text{CuO}_4$. AF=Antiferromagnetic, PM=Paramagnetic, I=Insulator, M=Metal, SG=SpinGlass, N=Normal, SC=Superconductor, T=tetragonal structure, O=Orthorhombic structure.

III. THE STARTING THEORETICAL MODEL

The band diagram shown in the figure 4 associated to the La_2CuO_4 was obtained by means of techniques of LAPW[13]. The last occupied band is half filled, predicting a metallic behavior, and its form suggests a Tight-Binding nature for the electron gas that occupied it within the effective environment of the rest of the bands. The less bound electrons to the compound La_2CuO_4 , are the ones of the Cu_2^+ atoms, that do not have closed their last shells (3d), at difference with the situation with the O_2^- ions. These electrons are the ones that form the last band in the corresponding solid.

The model proposed in the references [6, 7] is described in this section. One of the most used pictures to describe the movement of the valence electrons in a solid with a periodic potential is the tight-binding model. This model is applicable when the overlapping of the atomic orbitals of the neighbors can be considered small and it can be supposed that is not necessary to carry out significant corrections to the atomic wave functions, created by the interaction with the neighboring orbitals. The tight-binding approximation provides a reconciliation among the seemingly contradictory representations of the very localized atomic levels and on another hand the free electron model [14], in which the wave functions are lineal combination of planes waves.

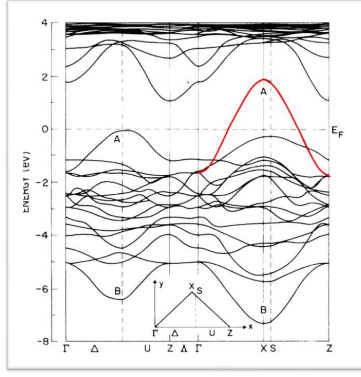


FIG. 4: Bands structure for the La_2CuO_4 calculated by Horsch y Stephan et.al. 1993. The semifilled band $\Gamma - X$ predict a tight-binding behavior in the reciprocal plane

From the previous comments we can suppose that these electrons are strongly correlated to the base cells CuO_2 , preferably toward the corresponding centers of Cu [15]. Then, the lattice will be supposed as the square lattice of Cu atoms located at the CuO planes (see figure 5).

The electrons not belonging to the last band and the nuclear charge that neutralizes them, play a double role. They act in one hand, as an effective polarizable medium that screens the field produced by a point charge external to them, and in second place, due to their spatial distribution and magnitude, they guarantee with their action the periodic order of the solid, that is modeled with a periodic potential in the lattice of points.

The Hamiltonian of the model introduced in the references take the form:

$$\hat{H} = \sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{i=1}^N W_\gamma(\vec{x}_i) + \sum_{i=1}^N F_b(\vec{x}_i) + \frac{1}{2} \sum_{i=1}^N \sum_{j \neq i}^N V(\vec{x}_i, \vec{x}_j) + \sum_{i=1}^N \hat{U}_{SO} \quad (1)$$

where $\frac{p_i^2}{2m}$ is the kinetic energy term, $W_\gamma(\vec{x}_i) = W_\gamma(\vec{x}_i + \vec{R})$ is the periodic potential that exercise the electrons in the partially filled single band, and \vec{R} runs over the points of the lattice of Cu (see figure 5),

$F_b(\vec{x}_i) = \sum_{\vec{R}} \int d^2y \frac{e^2}{4\pi\epsilon\epsilon_0} \frac{\exp(-\frac{|\vec{y}-\vec{R}|^2}{b^2})/\pi b^2}{|\vec{x}_i-\vec{y}|}$, $b \ll p$. is the potential of the jellium background correspondingly only to the surplus of charges which neutralize the electrons that partially filled the band,

$V(\vec{x}_i, \vec{x}_j) = \frac{e^2}{4\pi\epsilon\epsilon_0} \frac{1}{|\vec{x}_i-\vec{x}_j|}$ screened Coulomb potential,

$V(\vec{x}_i) = W_\gamma(\vec{x}_i) + F_b(\vec{x}_i)$ is the effective potential that feel the electrons that partially filling the last band,

$\hat{U}_{SO} = \frac{\hbar}{2m^2c^2} \nabla V(\vec{x}_i) \cdot \vec{\sigma} \times \hat{p}$ is the spin-orbit interaction term.

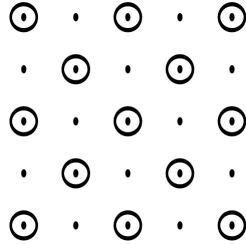


FIG. 5: Punctual lattice associated to the CuO planes. To obtain the AFM properties of the electronic gas, and more general, to release the symmetries restriction, it is separated the lattice in the 2 represented red

A. The Hartree-Fock method

One of the most useful techniques to find approximate solutions to the Schrodinger's equation is the molecular orbitals approximation. In this approach it is considered that the electrons occupy spin-orbital functions of a given energy. This technique is based in the *variational theorem*, which state that the expected value of \hat{H} for an arbitrary wave function is not smaller than the lowest eigenvalue E_0 corresponding to the exact solution of the equation[16]. Then, the best wave function is obtained when the energy calculated by the equation (2) has a minimum.

$$E = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}. \quad (2)$$

Then, the problem is reduced to find the solution by finding it form in all the allowed many electronic states, under the condition of making minimal the energy of the system. In the HF formalism one keeps each electron in a spin-orbital, in the field of the nucleus and the other electrons that are in their respective spin-orbitals (fixed), subject to the constraint that the spin-orbitals are orthonormal. After this minimization process, the HF equations for individual spin-orbitals result:

$$\hat{f}_i \phi_i = \varepsilon_i \phi_i, \quad (3)$$

where \hat{f}_i is the Fock operator and ε_i are the eigenvalues that represent the energies of the spin-orbitals (ϕ_i).

The Fock operator for an arbitrary electron '1' (equation 4) can be separated in three terms like it is shown next:

$$\hat{f}_i(1) = \hat{H}^0(1) + \sum_{i=1}^N [\hat{J}_i(1) - \hat{K}_i(1)], \quad (4)$$

where the Hamiltonian operator $\hat{H}^0(1)$ is defined by:

$$\hat{H}^0(1) = \frac{p_1^2}{2m} + W_\gamma(\vec{x}_1) + F_b(\vec{x}_1). \quad (5)$$

Here and in what follows, the arguments of the wave functions '1' and '2', indicate the collection formed by the spacial coordinates and the spin. In absence of interelectronic interactions (5) will be the only operator corresponding to the movement of a single electron in the field of the nucleus and the other electrons, that do not pertain to the partially filled band crossing the Fermi level.

The direct interaction operator is

$$\hat{J}_j(1)\phi_a(1) = \left\{ \int d\tau_2 \phi_j(2) \frac{e^2}{4\pi\epsilon\epsilon_0 r_{12}} \phi_j(2) \right\} \phi_a(1), \quad (6)$$

where $\int d\tau_2$ represents the integral for the space coordinates and the sum for the spin coordinates. This operator correspond to the average potential of an electron in the state ϕ_j .

On the other hand the exchange operator is expressed as:

$$\hat{K}_j(1)\phi_a(1) = \left\{ \int d\tau_2 \phi_j(2) \frac{e^2}{4\pi\epsilon\epsilon_0 r_{12}} \phi_a(2) \right\} \phi_j(1). \quad (7)$$

The equation (3) is known as the canonical HF equation and the fact that it corresponds to a non linear eigenvalue and eigenfunctions problem, implies that to find the solutions becomes necessary an iterative procedures. This fact leads to propose a group of test spin-orbitals that allow to obtain a new group of such orbitals, from which a new Fock operator is generated. The process is repeated until the energy and the functions converges, such a procedure is named the self-consistent field process.

B. The approximate basis functions

In a general way the spin-orbitals (ϕ_i) are expanded by means of a well-known group of basis functions associated with the geometric positions of the nuclei. This basis should satisfy two practical conditions

1. Should reasonably describe the physics of the problem.
2. The integrals that appears in the mathematical treatment should be evaluates with relative easiness.

The spatial components of the spin-orbitals is expanded in terms of the basis functions generally centered in atoms, according to (8). The expansion which must be infinite in principle, is truncated using a number of functions \mathbf{M} , being $c_{\nu i}$ the coefficients determining each atomic orbital contribution χ_ν in the linear expansion [17]

$$\phi_i = \sum_{\nu=1}^M c_{\nu i} \chi_\nu. \quad (8)$$

Substituting the orbitals expanded according to (8) in the HF equation [18], a set of matrix equations is obtained which can be:

$$\mathbf{F}\mathbf{C} = \mathbf{S}\mathbf{C}\varepsilon, \quad (9)$$

where \mathbf{F} is the Fock matrix for the $F_{\mu\nu} = \langle \chi_\mu | f | \chi_\nu \rangle$; \mathbf{S} is the superposition matrix among the elements of the base $S_{\mu\nu} = \langle \chi_\mu | \chi_\nu \rangle$ and \mathbf{C} is the coefficients matrix $c_{\nu i}$.

In the beginnings, the developing of HF techniques for systems of many particles, like bands and polyatomic complex calculations, was limited by the memory and speed of the machine calculators of that times. It was necessary to devise, on the basis of arguments and credible approaches, for example like the hole's Fermi model [19], mean field approximation, etc, a reduction of the functional space for searching and of the complications of the calculations. An useful assumption is to consider that the solution states of the system of equations(9) have quantized spin in the same direction in all the space, that is to say:

$$\phi_{\mathbf{k}}(x, s) = \begin{cases} \phi_{\mathbf{k}}^\alpha(x) u_\uparrow(s) & \text{type } \alpha \text{ state,} \\ \phi_{\mathbf{k}}^\beta(x) u_\downarrow(s) & \text{type } \beta \text{ state.} \end{cases} \quad (10)$$

If the spatial functions $\phi_{\mathbf{k}}^\alpha$ and $\phi_{\mathbf{k}}^\beta$ are identical, the HF calculations is named as restrictive, otherwise unrestricted [20]. However, due to their definitions, both cases are restrictive.

It can be said that the HF system of equations (9) is written in a form being invariant under rotation, because it is not considered the spin quantization in one absolute direction. That is, the states to be found are not α type neither β one. The first in derive the HF equations in this fully unrestricted form was P. A. M. Dirac in the 1930 [21]. Work in this rotation invariant way wide the functional space being investigated. In consequence it allows to extend the HF scheme towards the search of ground states showing magnetic character. This possibility is suggested in references [6, 7]. These works considered a base that allowed to find HF solutions for the spin-orbitals showing spin quantization depending of the spatial position.

The Tight-Binding basis in the one band approximation, that was used in these works consists of 4 sets of basis functions:

$$\varphi_{\mathbf{k}}^{(r, \sigma_z)}(\mathbf{x}, s) = \sqrt{\frac{2}{N}} u^{\sigma_z}(s) \sum_{\mathbf{R}^{(r)}} \exp(i\mathbf{k} \cdot \mathbf{R}^{(r)}) \varphi_0(\mathbf{x} - \mathbf{R}^{(r)}), \quad (11)$$

$$\hat{\sigma}_z u^{\sigma_z} = \sigma_z u^{\sigma_z}, \quad (12)$$

$$\varphi_0(\mathbf{x}) = \frac{1}{\sqrt{\pi a^2}} \exp\left(-\frac{\mathbf{x}^2}{2 a^2}\right), \quad (13)$$

where $a \ll p$, $r = 1, 2$ and $\sigma_z = \pm \frac{1}{2}$.

The equation (9) projected in the tight binding basis (11) was written in the form:

$$[H_{\mathbf{k}} + \tilde{\chi} (J_{\mathbf{k}} - K_{\mathbf{k}} - F_{\mathbf{k}})] \cdot \mathbf{B}^{\mathbf{k},l} = \tilde{\varepsilon}_l(\mathbf{k}) S_{\mathbf{k}} \cdot \mathbf{B}^{\mathbf{k},l}, \quad (14)$$

where $H_{\mathbf{k}}$ is Hamiltonian part that corresponds to the kinetic energy and the total effective potential, $J_{\mathbf{k}}$ is the direct interaction term,

$K_{\mathbf{k}}$ is the exchange term,

$F_{\mathbf{k}}$ it is the neutralizing bottom potential,

$S_{\mathbf{k}}$ is the overlapping matrix.

Also $\tilde{\chi} \equiv \frac{me^2 a}{4\pi\hbar^2 \epsilon \epsilon_0 p}$ and $\tilde{\varepsilon}_l(\mathbf{k}) \equiv \frac{ma^2}{\hbar^2} \varepsilon_l(\mathbf{k})$ are the dimensionless parameters in those that a is the characteristic radius of the functions φ_0 , $p = 3.8\text{\AA}$ is the separation between two Cu near neighbors in the absolute red, \hbar is Planck constant, m and e are the mass and the charge of the electron respectively.

In the low overlapping approximation among nearest neighbors (that is to say among different sublattices) the functions of the base that correspond to different sublattices with the same spin quantization are the only one, not being orthogonal. However, the orthogonalization of different elements of the same sublattice, as well as the unit norm of all elements, are valid. The $\varphi_0(\mathbf{x} - \mathbf{R}^{(r)})$ orbitals will be called as Wannier orbitals and represent the probability amplitude to find an electron in the surroundings of a point of the lattice.

IV. MAGNETICS PROPERTIES

Magnetism arises on the sub-atomic level from localized polarization of the electron clouds of certain atoms arising from unpaired electrons. This causes the charge on the atom to have a lattice angular momentum. Any flow of charge causes additional physical effects on the surroundings, usually referred to as a *magnetic* effect. In the case of atoms the lattice angular momentum of the charge cloud causes a magnetic field perpendicular to the rotation plane of the charge. The magnitude of this magnetic or spin moment is dependent on the species of atoms [22]. How these spin moments interact with each other is critical to how different materials are characterized magnetically. When atoms are brought in proximity to each other there is a probability of an electron jumping from one atom to another, known as the Heisenberg exchange [4]. This interaction probability can indirectly couple the spin moments of the atoms, causing the spin moments to align parallel or anti-parallel. In most materials the spin moments are small and aligned randomly, leading to paramagnetism as shown in Figure. In some materials however, specifically transition metals such as nickel, cobalt, and iron, the spin moments are large, and align in parallel. This causes a lattice spontaneous magnetic moment in the material.

In $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ case, the use of scattering of neutrons techniques [23], has contributed important information about the magnetic structure of these materials. In the figure 6 the AFM profile of the La_2CuO_4 in the copper-oxygen is shown. The places Cu contains the magnetic moment, whose address rests approximately to 45 grades on the link CuO. It happens that the ions O_2^- and La_3^+ complete their more external layers, while the Cu_2^+ lacks an electron for it. Then the ion Cu presents an electron without matching up. It is also the less bound one to the arrangement.

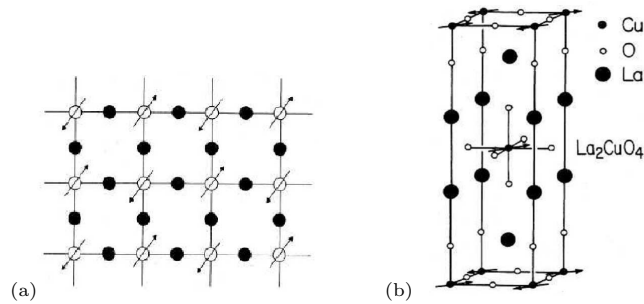


FIG. 6: (a) Magnetic structure of the $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. Schematic representation of the CuO_2 planes, the copper and the oxygen are represented by means of hollow and padded circles, respectively (b) Magnetic structure of the $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ in its planes CuO_2

V.

VI. ANISOTROPY ENERGY AND MAGNETOCRYSTALLINE ANISOTROPY

One of the most basic parameters in a magnetic system is the magneto-crystalline anisotropy, that is, the preference of the spin moments to align with some fixed crystallographic axes. This is a consequence of the interaction of the local environment through its spin-orbit interaction with the electrons. The simplest form of anisotropy is the uniaxial one that consists in that the magnetic moment prefers to align throughout a simple axis \vec{e} , usually called the easy axis.

Considering the operator $\sum_{i=1}^N \hat{U}_{SO}$ as an perturbation of the initial Hamiltonian 1, the anisotropy energy will be evaluated in this subsection, in the first correction to the HF energy of the system, according to the corresponding formula of perturbation theory.

$$E_{\text{anisotropy}}(\vec{n}, \theta) = \sum_{k,l} \langle \phi_{k,l}^R | \hat{U}_{SO} | \phi_{k,l}^R \rangle, \quad (15)$$

where the $|\phi_{k,l}^R\rangle$ orbitals are obtained of rotating the orbital solution $|\phi_{k,l}\rangle$ around the axis defined by the unitary vector \vec{n} in an angle θ . To rotate the orbital one should interpret the following procedure: Let us suppose that we have an orbital that is eigenfunctions of the operator $\hat{\sigma}_z$ and we make a rotation around the axis defined by the unitary vector \vec{n} in an angle θ . Then, the z axis will become an z' axis, and the orbital will be transformed in an orbital that is eigenfunction of $\hat{\sigma}_{z'}$ according to (16).

$$|\phi_{k,l}\rangle = \sum_{r,\sigma_z} B_{r,\sigma_z}^{k,l} |\varphi_{\mathbf{k}}^{(r,\sigma_z)}\rangle, \quad (16)$$

$$|\phi_{k,l}^R\rangle = U(a,b) |\phi_{k,l}\rangle, \quad (17)$$

$$U(a,b) = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}, \quad (18)$$

$$a = \cos\left(\frac{\phi}{2}\right) - in_z \sin\left(\frac{\phi}{2}\right), \quad (19)$$

$$b = -n_y \sin\left(\frac{\phi}{2}\right) - in_x \sin\left(\frac{\phi}{2}\right). \quad (20)$$

A rotation of the orbital leads to a rotation of the antiferromagnetic structure of the material at $T = 0$. This can be expressed in the following way [27]:

$$\vec{M}_R(\vec{x}) = \sum_{k,l} \langle \phi_{k,l}^R(\vec{x}) | \vec{\sigma} | \phi_{k,l}^R(\vec{x}) \rangle, \quad (21)$$

$$\vec{M}_R(\vec{x}) = \vec{\vec{R}} \sum_{k,l} \langle \phi_{k,l}(\vec{x}) | \vec{\sigma} | \phi_{k,l}(\vec{x}) \rangle, \quad (22)$$

$$\vec{M}_R(\vec{x}) = \vec{\vec{R}} \vec{M}(\vec{x}). \quad (23)$$

where $\vec{M}_R(\vec{x})$ is the magnetization vector rotated around an \vec{n} axis, in an angle θ starting from the initial direction of the magnetization vector $\vec{M}(\vec{x})$, and $\vec{\vec{R}}$ is the tensor that rotates the magnetization vector in the three-dimensional space.

The quantity $E_{\text{anisotrop-a}}(\vec{n}, \theta)$ can be interpreted in the following way: Let us suppose that the system has its antiferromagnetic structure in certain direction and that this structure is rotated around the axis \vec{n} in an angle θ . Then $E_{\text{anisotrop-a}}(\vec{n}, \theta)$ is the correction to the HF energy of the system produced by the spin-orbit interaction, when the magnetic structure has that direction (see figure 7).

VII. ANISOTROPY ENERGY WITH GAUSSIAN WANNIER ORBITALS

The anisotropy energy was studied in the initial model. That is, considering as the basis functions, the Bloch functions constructed in the sublattices by means of defined by Wannier Gaussian orbitals. It was already seen that in this two-dimensional model the spin-orbit operator reduces to the following form:

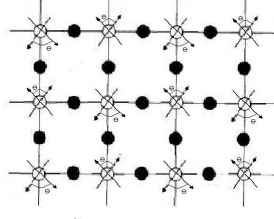


FIG. 7: Antiferromagnetic structure in the CuO planes rotated around the z axis in an angle θ .

$$\hat{U}_{SO} = -\frac{\hbar}{2m^2c^2}\hat{\sigma}_z \cdot (E_x\hat{p}_y - E_y\hat{p}_x). \quad (24)$$

In the following developments, it will be considered that $g = -\frac{\hbar}{2mc^2}$, where m is the electron mass. The expression for the energy to evaluate is given for:

$$E(\vec{n}, \theta) = \sum_{k,l} \langle \phi_{k,l}^R | \hat{U}_{SO} | \phi_{k,l}^R \rangle, \quad (25)$$

where $B_{r,\sigma_z}^{k,l}$ are the constants for the expansion of the HF solutions of the original problem in terms of the basis functions [6].

$$|\varphi_{\mathbf{k}}^{(r,\sigma_z)}(\vec{x}, s)\rangle = \sqrt{\frac{2}{N}} u^{\sigma_z}(s) \sum_{\vec{R}^{(r)}} \exp(i\mathbf{k} \cdot \vec{R}^{(r)}) \varphi_0(\vec{x} - \vec{R}^{(r)}).$$

The formula (25) can be wrote as follows:

$$E(\vec{n}, \theta) = g \sum_{k,l} \sum_{r,\sigma_z} \sum_{t,\alpha_z} B_{r,\sigma_z}^{k,l} B_{t,\alpha_z}^{k,l} f_{\alpha_z,\sigma_z}(\vec{n}, \theta) g(r, t), \quad (26)$$

$$f_{\alpha_z,\sigma_z}(\vec{n}, \theta) = u^{\alpha_z} U^+ \sigma_z U u^{\sigma_z},$$

$$g(r, t) = \frac{2}{N} \sum_{R^r, R^t} e^{i\mathbf{k} \cdot (\vec{R}^r - \vec{R}^t)} \int d^2\vec{x} \varphi_0(\vec{x} - \vec{R}^t) [E_x\hat{p}_y - E_y\hat{p}_x] \varphi_0(\vec{x} - \vec{R}^r).$$

In the nearest neighbor approximation, the term $g(r, t)$ take the following form:

$$g(r, t) = \begin{cases} \int d^2\vec{x} \varphi_0(\vec{x}) [E_x\hat{p}_y - E_y\hat{p}_x] \varphi_0(\vec{x}) & \text{if } r=t \\ \sum_{n=-1}^1 e^{ik_x np} \int_{V_2^n} d^2\vec{x} \varphi_0(\vec{x} + \vec{e}_x np) [E_x\hat{p}_y - E_y\hat{p}_x] \varphi_0(\vec{x}) + \\ \exp^{ik_y np} \int_{V_3^n} d^2\vec{x} \varphi_0(\vec{x} + \vec{e}_y np) [E_x\hat{p}_y - E_y\hat{p}_x] \varphi_0(\vec{x}) & \text{if } r \neq t \end{cases} \quad (27)$$

that can be expressed in more explicit form according to:

$$g(r, t) = \begin{cases} A \int d^2\vec{x} e^{-\frac{\vec{x}^2}{2a^2}} [E_yx - E_xy] e^{-\frac{\vec{x}^2}{2a^2}} & \text{if } r=t \\ \sum_{n=-1}^1 e^{ik_x np} \int_{V_2^n} d^2\vec{x} e^{-\frac{|\vec{x} + \vec{e}_x np|^2}{2a^2}} [E_yx - E_xy] e^{-\frac{\vec{x}^2}{2a^2}} + \\ e^{ik_y np} \int_{V_3^n} d^2\vec{x} e^{-\frac{|\vec{x} + \vec{e}_y np|^2}{2a^2}} [E_yx - E_xy] e^{-\frac{\vec{x}^2}{2a^2}} & \text{if } r \neq t \end{cases} \quad (28)$$

where $\varphi_0(\vec{x}) = \frac{1}{\sqrt{\pi a^2}} \exp(-\frac{\vec{x}^2}{2a^2})$ and $A = \frac{-\hbar i}{\pi a^4}$.

The integration regions are taken in what follows of fixed dimensions because the Wannier orbitals are very much localized in the Cu lattice centers. ($a = 0.25 p$, $p = 3.8 A^0$):

$$V_1 = (x, y) | -\frac{p}{2} < x, y < \frac{p}{2},$$

$$V_2^{+1} = (x, y) | -\frac{p}{2} < x < \frac{p}{2}, -\frac{3p}{2} < y < \frac{p}{2},$$

$$V_2^{-1} = (x, y) | -\frac{p}{2} < x < \frac{p}{2}, -\frac{p}{2} < y < \frac{3p}{2},$$

$$V_3^{+1} = (x, y) | -\frac{3p}{2} < x < \frac{p}{2}, -\frac{p}{2} < y < \frac{p}{2},$$

$$V_3^{-1} = (x, y) | -\frac{p}{2} < x < \frac{3p}{2}, -\frac{p}{2} < y < \frac{p}{2}.$$

As the Wannier orbitals are two-dimensional Gaussian functions, they coincide with the wavefunctions of the Harmonic two-dimensional oscillator. Therefore, from the analysis already done, we can easily derive the effective potential in the vicinity of the Cu as a parabolic potential (figure 8).

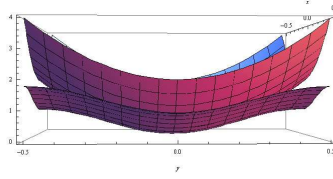


FIG. 8: Parabolic potential (up) and effective potential (down) that coincide in the vicinity of the Cu atoms. The unit of energy is $E = 8.3 eV$ and the length unit $p = 3.8 A^0$.

The components E_x , E_y of the electric field are derived from the effective potential, see figure 9. They are odd functions in the x, y coordinates, a property that makes that the integral factor $E_y x - E_x y$ is an odd function. As the integration regions are symmetrical regarding, at least one of the coordinates, it follows that $g(r, t) = 0$.

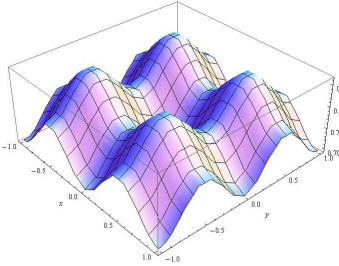


FIG. 9: Effective potential with the order symmetry equal to 4 of the crystalline lattice, with parabolic form around the Cu atoms, Gaussian Wannier orbitals. The unit of energy is $E = 8.3 eV$ and the length unit $p = 3.8 A^0$.

This result evidences that the Gaussian Wannier orbitals in our small overlapping approximation, predict a vanishing anisotropy energy. This means that the first correction to the HF energy for the system, determined by the spin-orbit interaction doesn't determine an easy magnetization axis. This result is not coinciding with the observations, which indicates the existence an easy axis at zero doping and $T = 0$. However, this difference can be attributed to various factors. One of them is the known absence of long range order in the pure 2D systems. Another cause, can be the fact that the model slightly simplifies the microscopic structure of the electron system by assuming it as pure two dimensional and moreover, by considering Wannier orbitals not resembling open the shell properties of the Cu atoms.

The reduced form of $g(r, t)$ (27) indicates that their value only depends on the properties of symmetry of the electric field and the orbitals in a vicinity of the Cu, and not in the whole lattice. It points that out is fundamental to more deeply formulate the starting basis of states for the model to predict the magnetic properties.

VIII. ANISOTROPY ENERGY WITH WANNIER ORBITALS BEING ODD OR EVEN FUNCTIONS

In this section, it is considered a modification of the orbitals of the model in reference [6, 7]. It is supposed that the Wannier orbitals are three-dimensional. Their symmetry is assumed with the same properties as the original problem. The Wannier orbitals in general sense will be denoted by $\psi(x_1, x_2, x_3)$. It is supposed that they are even or odd functions regarding the inversion of anyone of their coordinates, referred to the Cu atoms in that they are centered. In this case the spin-orbit operator should have the usual form in three dimensions :

$$\hat{U}_{SO} = -\frac{\hbar}{2m^2c^2}[\hat{\sigma}_x \cdot (\partial_y V \hat{p}_z - \partial_z V \hat{p}_y) + \hat{\sigma}_y \cdot (\partial_z V \hat{p}_x - \partial_x V \hat{p}_z) + \hat{\sigma}_z \cdot (\partial_x V \hat{p}_y - \partial_y V \hat{p}_x)]. \quad (29)$$

From the definition of the anisotropy energy (15) and (29), it follows that it is a lineal combination of terms of the form:

$$E(\vec{n}, \theta) = \sum_{i=1, j=1, i \neq j}^3 (A_{ij} H_{ij0} + B_{ij+} H_{ij1+} + B_{ij-} H_{ij1-} + C_{ij+} H_{ij2+} + C_{ij-} H_{ij2-}), \quad (30)$$

where the $H_{ijk\pm}$ are of the following form:

$$\begin{aligned} H_{ij0} &= \int_{V_0} dx_1 dx_2 dx_3 \psi(x_1, x_2, x_3) E_{x_i} \hat{p}_j \psi(x_1, x_2, x_3), \\ H_{ij1\pm} &= \int_{V_{1\mp}} dx_1 dx_2 dx_3 \psi(x_1 \pm p, x_2, x_3) E_{x_i} \hat{p}_j \psi(x_1, x_2 \pm p, x_3), \\ H_{ij2\pm} &= \int_{V_{2\mp}} dx_1 dx_2 dx_3 \psi(x_1, x_2 \pm p, x_3) E_{x_i} \hat{p}_j \psi(x_1 \pm p, x_2, x_3), \end{aligned}$$

where the regions of integration $V_1, V_{3x\mp}, V_{2y\mp}$ can have in general sense three possible spatial symmetries, when are defined by:

$$\begin{aligned} V_0 &= (x, y, z) | -\frac{p}{2} < x, y < \frac{p}{2}, -\frac{h}{2} < z < \frac{h}{2}, \\ V_{1+} &= (x, y, z) | -\frac{p}{2} < x < \frac{3}{2}\frac{p}{2}, -\frac{p}{2} < y < \frac{p}{2}, -\frac{h}{2} < z < \frac{h}{2}, \\ V_{1-} &= (x, y, z) | -\frac{3}{2}\frac{p}{2} < x < \frac{p}{2}, -\frac{p}{2} < y < \frac{p}{2}, -\frac{h}{2} < z < \frac{h}{2}, \\ V_{2+} &= (x, y, z) | -\frac{p}{2} < x < \frac{p}{2}, -\frac{p}{2} < y < \frac{3}{2}\frac{p}{2}, -\frac{h}{2} < z < \frac{h}{2}, \\ V_{2-} &= (x, y, z) | -\frac{p}{2} < x < \frac{p}{2}, -\frac{3}{2}\frac{p}{2} < y < \frac{p}{2}, -\frac{h}{2} < z < \frac{h}{2}. \end{aligned}$$

Next it follows that:

$$\int_{V_0} dx_1 dx_2 dx_3 \psi(x_1, x_2, x_3) E_{x_i} \hat{p}_j \psi(x_1, x_2, x_3) = 0, \quad (31)$$

$$\int_{V_{1\mp}} dx_1 dx_2 dx_3 \psi(x_1 \pm p, x_2, x_3) E_{x_i} \hat{p}_j \psi(x_1, x_2 \pm p, x_3) = 0, \quad (32)$$

$$\int_{V_{2\mp}} dx_1 dx_2 dx_3 \psi(x_1, x_2 \pm p, x_3) E_{x_i} \hat{p}_j \psi(x_1 \pm p, x_2, x_3) = 0. \quad (33)$$

It can be underlined that the two functions $p(x_1, x_2, x_3)$ and $t(x_1, x_2, x_3)$ have the same parity regarding x_i if both are even or odd.

It is considered in our analysis that the effective potential near the Cu atoms of our model is even. Hence it follows that the fields $E_{x_i} = -\partial_{x_i} V$ are odd functions regarding x_i and once fixed x_i , is even regarding the others coordinates $x_{j,k}$.

Let us show the (31-33) properties now.

Proof of 31.

1. The functions $\psi(x_1, x_2, x_3)$ and $\partial_{x_j}\psi(x_1, x_2, x_3)$ has the same parity regarding x_i and using the initial premise about the fields, the integrand is an odd function concerning the x_i coordinate.
2. Let us use the result: If the integral of a function converges absolutely, in an integration region in R^3 that has parallelepiped form, then the iterate integrals can commute the integration order (Theorem of Fubini).
3. Using the previous result we concluded that $\int_{V_0} dx_1 dx_2 dx_3 \psi(x_1, x_2, x_3) E_{x_i} \hat{p}_j \psi(x_1, x_2, x_3) = 0$

Proof of 32.

1. If $x_i = x_1$, then $\psi(x_1, x_2, x_3)$ and $\partial_{x_j}\psi(x_1 \pm p, x_2, x_3)$ have different parity regarding x_j and E_{x_i} and continues being even regarding x_j , of the initial premise, for what (32) is kept.
2. If $x_i = x_{2,3}$, $\psi(x_1, x_2, x_3)$ and $\partial_{x_j}\psi(x_1 \pm p, x_2, x_3)$ have identical parity regarding x_i and using the initial premise of the fields, then the integrand is odd regard the x_i coordinate, for that (32) is kept.
3. In both cases the before cited Fubini property was employed.

Proof of 33

1. If $x_i = x_2$, it follows that $\psi(x_1, x_2, x_3)$ and $\partial_{x_j}\psi(x_1, x_2 \pm p, x_3)$ have different parity regard x_j , and E_{x_i} continues been even regard x_j , of the initial premise, for what it vanishes.
2. If $x_i = x_{1,3}$, $\psi(x_1, x_2, x_3)$ and $\partial_{x_j}\psi(x_1, x_2 \pm p, x_3)$ have identical parity regard x_i and using the initial premise of the fields, then has an odd integrand regard the x_i coordinate, and (33) is kept.
3. In both cases the result of Fubini also was used.

The results are summarized in the following form: If the Wannier orbitals that we propose are even or odd functions regard the space coordinates and the effective potential that it is assumed in the vecinity of the Cu atoms, is an even function regards the space coordinates, the anisotropy energy in the model also vanishes and therefore an axis easy magnetization is not predicted. Notice that the condition, that Wannier orbitals that we propose are even or odd functions, is enough but not necessary condition for the vanishing of the energy. This fits the possibility that using orbitals that neither be even or odd, a non vanishing anisotropy energy could follows.

As it is known that the less bound electrons of the Cu_2^+ occupy the d orbitals, and the electrons $\text{Cu}_2 +$ considered into our model, are representing the one partially filling the most energetic band in La_2CuO_4 , we can expect that the Wannier orbitals of our problem should more closely resemble the $d_{x^2-y^2}$ orbitals of Cu . These $d_{x^2-y^2}$ orbitals are solutions of the hydrogen atom,. Then, we could assume as the potential in the vicinities of the Cu a Coulomb potential alternatively as it was considered in the initial model. The Wannier orbitals of the $d_{x^2-y^2}$ type are even functions regarding the space coordinates. The components of the electric field E_{x_i} are odd functions because derived of the coulomb potential. Then we uses the previous result to conclude that, if we suppose orbitals of the $d_{x^2-y^2}$ type then the model again will predicts anisotropy energy null and non easy axis of magnetization. However, the possibility of employing a general linear combination of the d orbitals of Cu in addition to a more realistic 3D character of the model by including multiple CuO planes, opens the the opportunity to describe the observed antiferromagnetic anisotropy at low doping and temperatures.

IX. SPIN-ORBIT OPERATOR IN THE HARTREE-FOCK APPROXIMATION

To study the influence of the spin-orbit operator in the Hartree-Fock approximation the operator is projected in the basis of the orbitals proposed in the model:

$$[\mathbf{H}_{\mathbf{k}} + \tilde{\chi} (\mathbf{J}_{\mathbf{k}} - \mathbf{K}_{\mathbf{k}} - \mathbf{F}_{\mathbf{k}})] \cdot \mathbf{B}^{\mathbf{k},l} = \tilde{\varepsilon}_l(\mathbf{k}) S_{\mathbf{k}} \cdot \mathbf{B}^{\mathbf{k},l}. \quad (34)$$

We can include the spin operator to obtain the next matrix equation

$$[\mathbf{H}_{\mathbf{k}} + \hat{\mathbf{U}}_{\mathbf{k}}^{SO} + \tilde{\chi} (\mathbf{J}_{\mathbf{k}} - \mathbf{K}_{\mathbf{k}} - \mathbf{F}_{\mathbf{k}})] \cdot \mathbf{B}^{\mathbf{k},l} = \tilde{\varepsilon}_l(\mathbf{k}) S_{\mathbf{k}} \cdot \mathbf{B}^{\mathbf{k},l}, \quad (35)$$

where the derivation of the term $\hat{\mathbf{U}}_{\mathbf{k}}^{SO}$ in the model is presented next:

$$\begin{aligned}
\langle \varphi_{\mathbf{k}}^{(t,\alpha_z)}(\vec{x}, s) | \hat{U}_{SO} | \phi_{k,l} \rangle &= \langle \varphi_{\mathbf{k}}^{(t,\alpha_z)}(\vec{x}, s) | A \hat{\sigma}_z (E_x \hat{p}_y - E_y \hat{p}_x) \sum_{r,\sigma_z}^{r,\sigma_z} B_{r,\sigma_z}^{k,l} | \varphi_{\mathbf{k}}^{(r,\sigma_z)} \rangle, \\
\langle \varphi_{\mathbf{k}}^{(t,\alpha_z)}(\vec{x}, s) | \hat{U}_{SO} | \phi_{k,l} \rangle &= \sum_{r,\sigma_z}^{r,\sigma_z} \langle \varphi_{\mathbf{k}}^{(t,\alpha_z)}(\vec{x}, s) | A \hat{\sigma}_z (E_x \hat{p}_y - E_y \hat{p}_x) | \varphi_{\mathbf{k}}^{(r,\sigma_z)} \rangle B_{r,\sigma_z}^{k,l},
\end{aligned}$$

where $A = -\frac{\hbar}{2m^2c^2}$

$$\hat{U}_{\mathbf{k}}^{SO} = A \langle \varphi_{\mathbf{k}}^{(t,\alpha_z)}(\vec{x}, s) | \hat{\sigma}_z (E_x \hat{p}_y - E_y \hat{p}_x) | \varphi_{\mathbf{k}}^{(r,\sigma_z)} \rangle,$$

$$\hat{U}_{\mathbf{k}}^{SO} = A \frac{2}{N} \sigma_z \delta_{\alpha_z, \sigma_z} \sum_{\vec{R}^{(r)}, \vec{R}^{(t)}} e^{i\vec{k}(\vec{R}^{(t)} - \vec{R}^{(r)})} \int \varphi_0(\vec{x} - \vec{R}^{(t)}) (E_x \hat{p}_y - E_y \hat{p}_x) \varphi_0(\vec{x} - \vec{R}^{(r)}).$$

In the near neighbor approximation the term $\hat{U}_{\mathbf{k}}^{SO}$ take the following form:

$$\hat{U}_{\mathbf{k}}^{SO} = A \sigma_z \delta_{\alpha_z, \sigma_z} [\delta_{t,r} I_1 + (\delta_{t-1,r} + \delta_{t,r-1}) (e^{ik_1 p} I_{-2} + e^{-ik_1 p} I_{+2} + e^{ik_2 p} I_{-3} + e^{-ik_2 p} I_{+3})],$$

$$I_1 = \int_{V_1} d^2 \vec{x} \varphi_0(\vec{x}) (E_x \hat{p}_y - E_y \hat{p}_x) \varphi_0(\vec{x}),$$

$$I_{\mp 2} = \int_{V_{\mp 3}} d^2 \vec{x} \varphi_0(\vec{x} \mp p \vec{e}_x) (E_x \hat{p}_y - E_y \hat{p}_x) \varphi_0(\vec{x}),$$

$$I_{\mp 3} = \int_{V_{\mp 2}} d^2 \vec{x} \varphi_0(\vec{x} \mp p \vec{e}_y) (E_x \hat{p}_y - E_y \hat{p}_x) \varphi_0(\vec{x}).$$

For the same reasons that in section (anisotropy energy with orbitals of Wannier gaussian) the five integrals are null.

$$I_1 = I_{\mp 2} = I_{\mp 3} = 0 \implies \hat{U}_{\mathbf{k}}^{SO} = 0.$$

We can conclude that the spin-orbit operator is null in the matrix Hartree Fock representation, that implies no change in the Hartree Fock solution.

The same analysis could be done with the three dimensional Wannier orbitals and the result using the section (Anisotropy energy with orbitals of Wannier that are odd or even functions) would be the same as for bidimensional Gaussian Wannier orbitals.

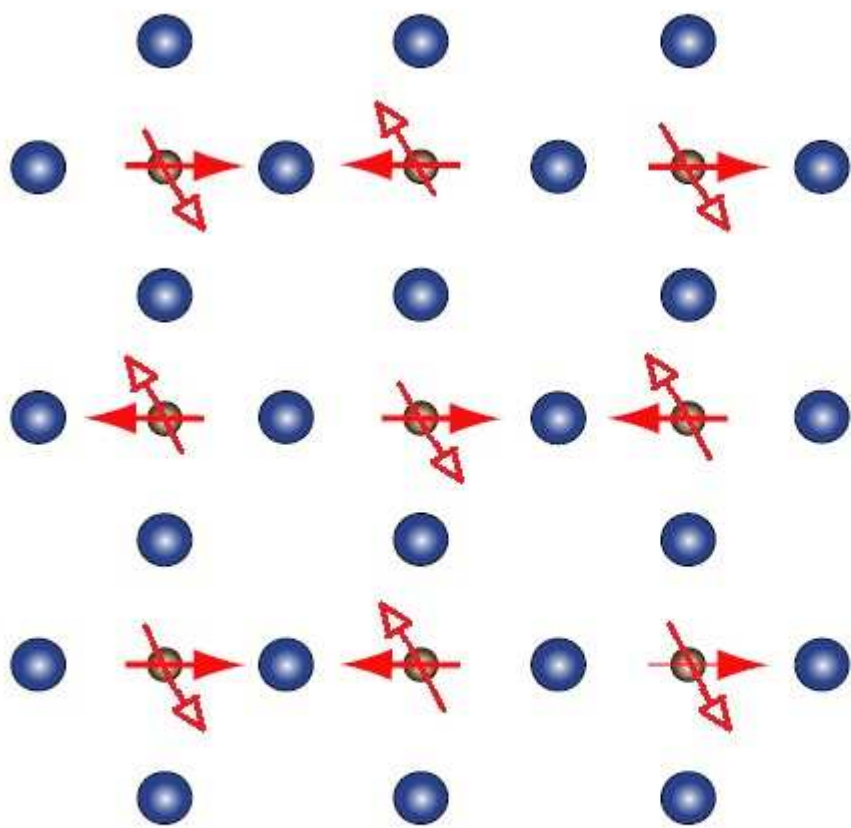
X. SUMMARY

We have studied the magnetic anisotropy properties of La_2CuO_4 at zero temperature, in the context of a two-dimensional model of the layers CuO, which Hartree Fock solutions were obtained in references[6]. For this purpose the spin-orbit interaction was considered as a perturbation to the initial Hamiltonian of the system and the energy was evaluated as a function of the direction of the antiferromagnetic structure of the material, when it is rotated. The basic conclusions of the work are:

- 1) The magnetic anisotropy energy strongly depends on the space dependence of the orbitals of Wannier and the effective potential that the electrons feel in the proximity of Cu.
- 2) For the Gaussian Wannier orbitals and their parabolic corresponding effective potential employed in the model, it was obtained that the magnetic anisotropy energy vanishes. Then, an easy axis of magnetization doesn't appears and the antiferromagnetic structure doesn't align in any direction.
- 3) The use of more general Wannier orbitals, as can be Gaussian atomic three-dimensional or orbital d type, assuming that they are even or odd, all produce vanishing anisotropy energy. This follows mainly because the orbitals and the potentials are even or odd functions with regard the coordinates.
- 4) The approach employed, that only considers non null overlapping among orbitals that are centered in near neighbors, is central in the previous conclusions.

- 5) The fact that the lattice of the Cu atoms is squared, strongly influences these results of zero magnetic anisotropy energy.
- 6) Wannier orbitals that are not spatially even neither odd, can predict non zero values of the magnetic anisotropy energy.

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